**2018 IMAG Futures Meeting – Moving Forward with the MSM Consortium (March 21-22, 2018)**

*Pre-Meeting Abstract Submission Form*

*\*Please submit to the NIBIB IMAG mailbox (*[NIBIBimag@mail.nih.gov](mailto:NIBIBimag@mail.nih.gov)*) by* ***January 8th, 2018***

*\*Save your abstract as “MSM PI Last Name \_ 2018 IMAG Futures Pre-Meeting Abstract”*

**PI(s) of MSM U01: Walter F. Boron, Emad Tajkhorshid, Erkki Somersalo**

**Institution(s): Case Western Reserve University, University of Illinois Urbana-Champaign**

**MSM U01 Grant Number: U01 GM111251**

**Title of Grant:** Multi-scale modeling of gas transport through channels in living cells

**Abstract**

Which MSM challenges are you addressing from the IMAG 2009 Report and how?

<https://www.imagwiki.nibib.nih.gov/content/2009-imag-futures-report-challenges>

(indicate which challenge (#) you’re addressing)

*You may insert images by copying and pasting below*

1: The project links respiratory, cardiovascular, and acid-base physiology.

3: The project is developing computation methods that link data-rich atomic data and data-rich macroscopic (cellular) data to predict behavior at the mesoscopic level.

6: The models in the projects drive new cell-physiology experiments.

8: The molecular dynamics (MD) modeling requires high-performance computing.

9: A goal is for predictions of the model (which will be available via a GUI) to drive physiological experiments that test and validate the model.

10. The methodologies for solving the computational models incorporate uncertainty quantification.

Are you using machine learning and or causal inference methods and how?

*You may insert images by copying and pasting below*

No.

Please briefly describe significant MSM achievements made (or expected).

*You may insert images by copying and pasting below*

We are developing a multi-scale modeling framework of gas permeation through protein channels in the cell membrane. The model integrates multiple scales in time (ns to s) and space (sub-nanometer to millimeter). At one extreme, we are using MD methods to model the movement of CO2 and H2O through individual aquaporin (AQP) tetramers. We also are developing novel computational methods to address the challenges of solving the model system at different scales in time and space. A particularly novel subproject is to model the microenvironment beneath the pH microelectrode used to collect surface-pH data (pHS) for a single cell that is exposed to CO2. The goal is to use the pHS data to extract the contribution of AQP channels to CO2 permeability. Finally, we are developing a GUI that will allow non-specialists to run simulations of their physiological experiments.

Please suggest any new MSM challenges that should be addressed by the MSM Consortium moving forward.

*You may insert images by copying and pasting below*

1. Mesoscopic models that link the atomic level to the cellular level. (2) Bring more experimentalists into the IMAG community to (a) inform the modelers of the important experimental questions that need to be addressed and also (b) educate the experimentalists on the power of computational models.

What expertise are on your team (e.g. engineering, math, statistics, computer science, clinical, industry) and who?

*Please list as “Expertise – Name, email”*

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